



**SEMMELWEIS
UNIVERSITY**



**PÁZMÁNY PÉTER
CATHOLIC UNIVERSITY**



Development of Complex Curricula for Molecular Bionics and Infobionics Programs within a consortial* framework**

Consortium leader

PÁZMÁNY PÉTER CATHOLIC UNIVERSITY

Consortium members

SEMMELWEIS UNIVERSITY, DIALOG CAMPUS PUBLISHER

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**Molekuláris bionika és Infobionika Szakok tananyagának komplex fejlesztése konzorciumi keretben

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WORLD OF MOLECULES

(Molekulák világa)

INTRODUCTION

(Bevezető)

KRISTÓF IVÁN



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Periodic system of elements

1. History of elements
2. Rutherford's scattering experiment
3. Bohr-Sommerfeld model
4. Elementary particles
5. Fundamental interaction
6. Periodic system/table of elements

Periodic system of elements

		Group																	
		I	II											III	IV	V	VI	VII	VIII
Period	1	1 H																	2 He
	2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
	3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
	4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
	5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
	6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
	7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo
	8	119 Uun																	
* Lanthanides		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu			
** Actinides		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr			

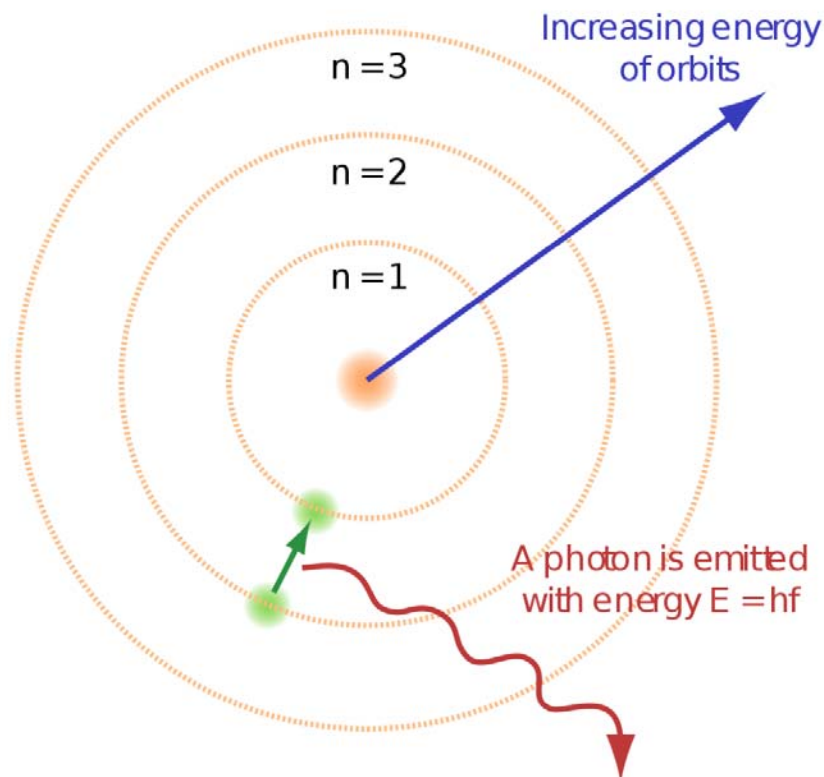
http://en.wikipedia.org/wiki/Periodic_table



Properties of atoms

1. Nucleus
2. Isotopes
3. Tables of isotopes
4. Radioactivity
5. Decay modes
6. Bohr-Sommerfeld model
7. Quantum numbers
8. Electron structure
9. Examples

Properties of atoms



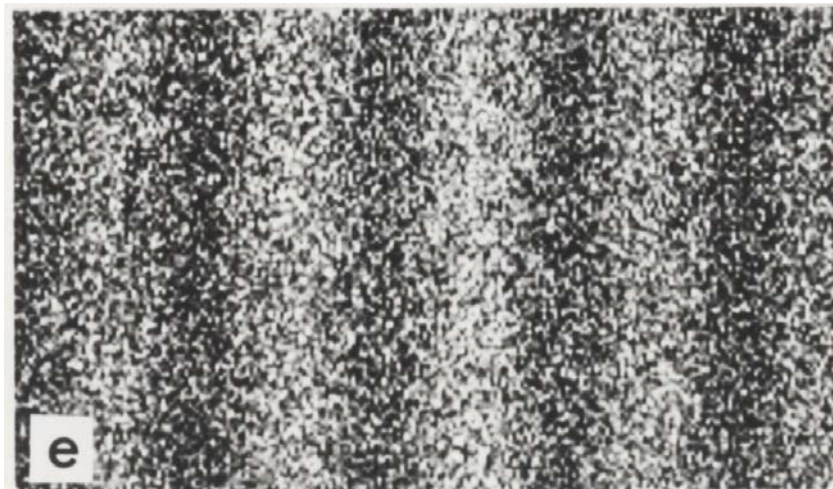
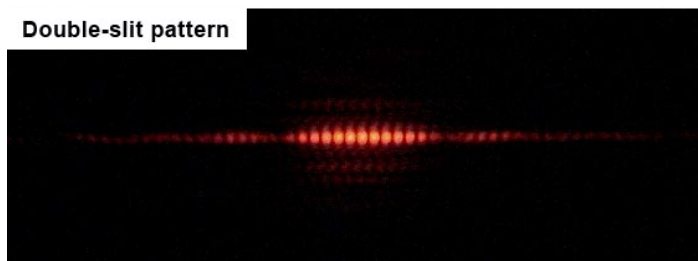
http://en.wikipedia.org/wiki/File:Bohr_atom_model_English.svg



Dual nature of electrons

1. Dual nature of light
2. Particle nature of electron
3. Wave nature of electrons (de Broglie)
4. Particle-wave duality of electrons
5. Schrödinger equation
6. The wave functions of the electron in 1D
7. The wave functions of the electron in a harmonic oscillator
8. The wave functions of the electron in 3D
9. The wave functions of the electron in the Hydrogen atom
10. Short introduction to complex numbers

Dual nature of electrons



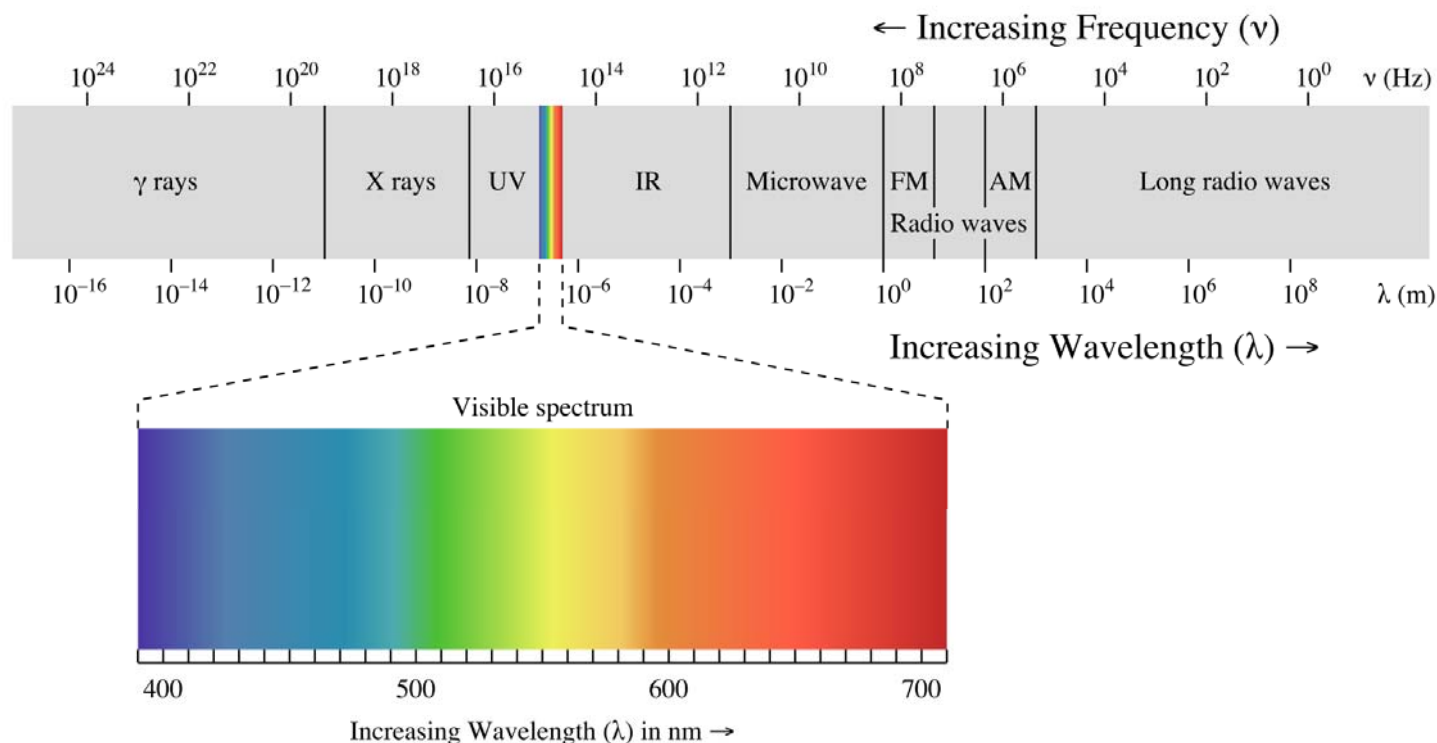
http://en.wikipedia.org/wiki/File:Single_slit_and_double_slit2.jpg
http://en.wikipedia.org/wiki/File:Double-slit_experiment_results_Tanamura_2.jpg



Properties of chemical bonds, spectroscopy

1. Spectroscopy
2. Absorption spectroscopy
3. Emission spectroscopy
4. Chemical properties of atoms
5. Types of chemical bondings
6. Basic properties of chemical bonds
7. Covalent, ionic and metallic bonds
8. Hydrogen bonds
9. van der Waals forces

Properties of chemical bonds, spectroscopy



http://en.wikipedia.org/wiki/File:EM_spectrum.svg

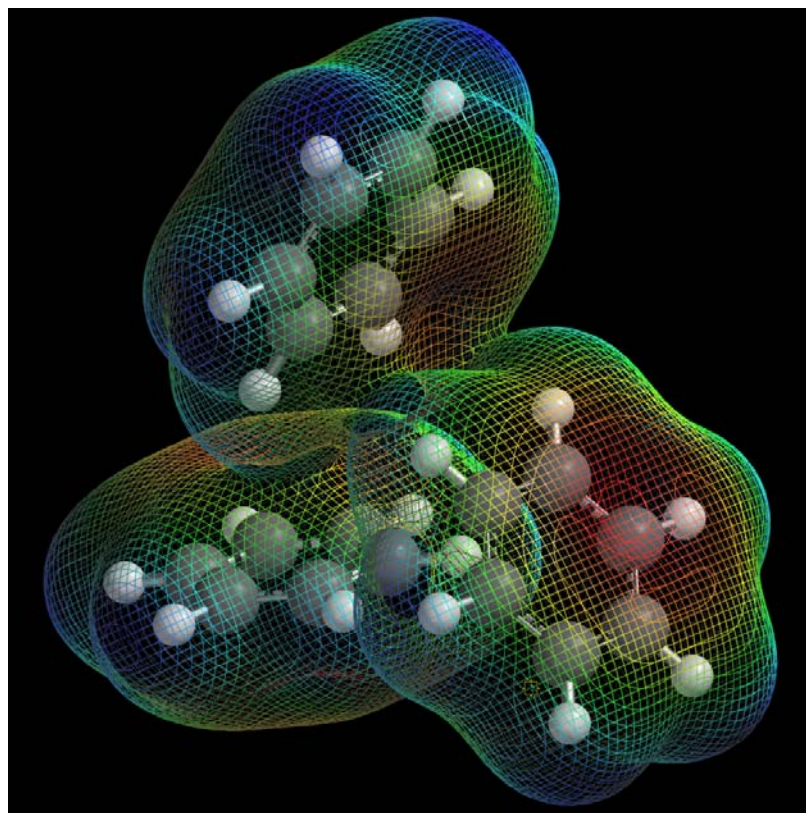


Modeling of electron and molecular structure

1. Modeling of the molecular and electron structure
2. Different methods
3. MM
4. Hartree-Fock
5. Semi-empirical
6. DFT
7. Møller Plesset
8. Approximations
9. Display options and methods



Modeling of electron and molecular structure



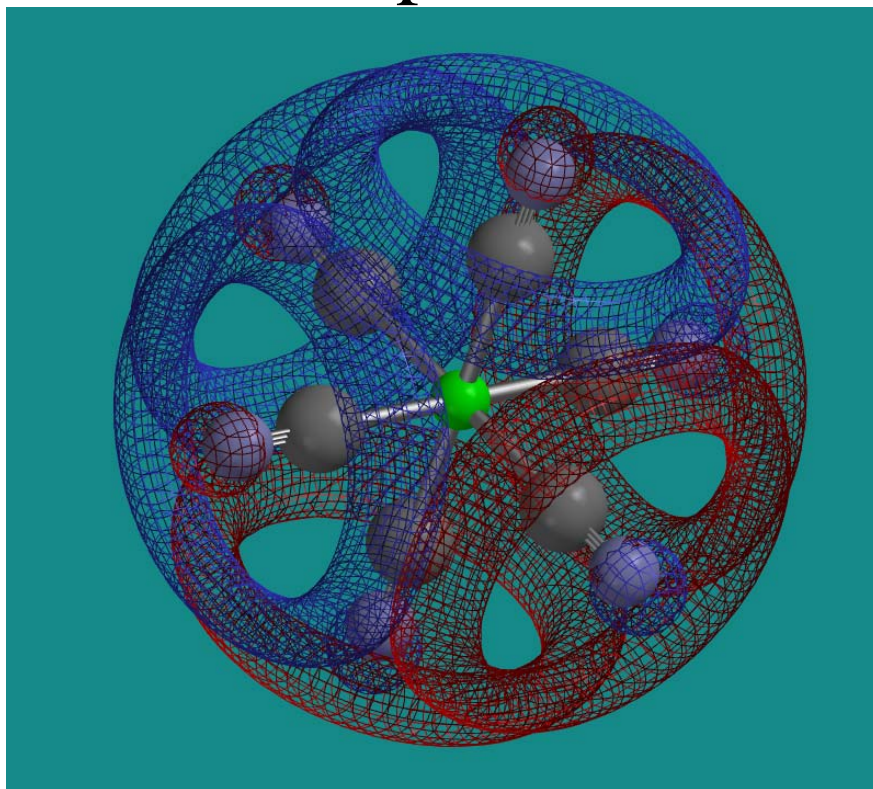


Chemical compounds, stoichiometry

1. Compounds
2. Chemical composition
3. Ambiguity of the chemical formula
4. Stoichiometry
5. Main groups of chemical compounds
6. Grouping of inorganic compounds
7. Salts
8. Properties of water



Chemical compounds, stoichiometry



ferrocyanide ion
 $[\text{Fe}(\text{CN})_6]^{4-}$
with LUMO+ orbitals plotted



Chemical equilibria, acid-base theories

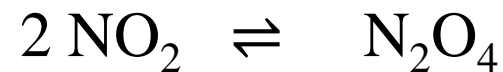
1. Chemical equilibria
 - equilibria in gases
 - acid-base equilibria
2. Acid-base theories
 - Arrhenius theory
 - Brønsted-Lowry theory
 - Lewis theory
 - Pearson theory (HSAB)
3. Superacids and superbases



Chemical equilibria, acid-base theories



the equilibrium reaction
of



left: hot, more NO_2

right: cold, more N_2O_4

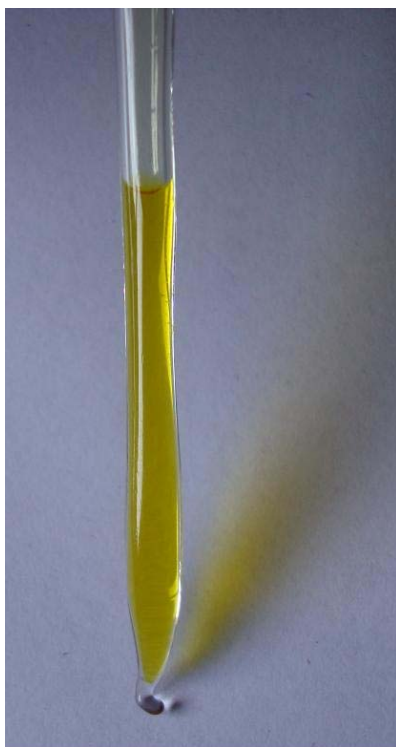
<http://commons.wikimedia.org/wiki/File:NO2-N2O4.jpg>



Case studies

1. Hydrogen,
2. Oxygen,
3. Carbon,
4. Nitrogen,
5. Sulphur,
6. Sodium,
7. Silicon,
8. Boron,
9. ...

Case studies



http://commons.wikimedia.org/wiki/File:Chlor_1a.jpg | http://de.wikipedia.org/w/index.php?title=Datei:Rock_salt_crystal.jpg

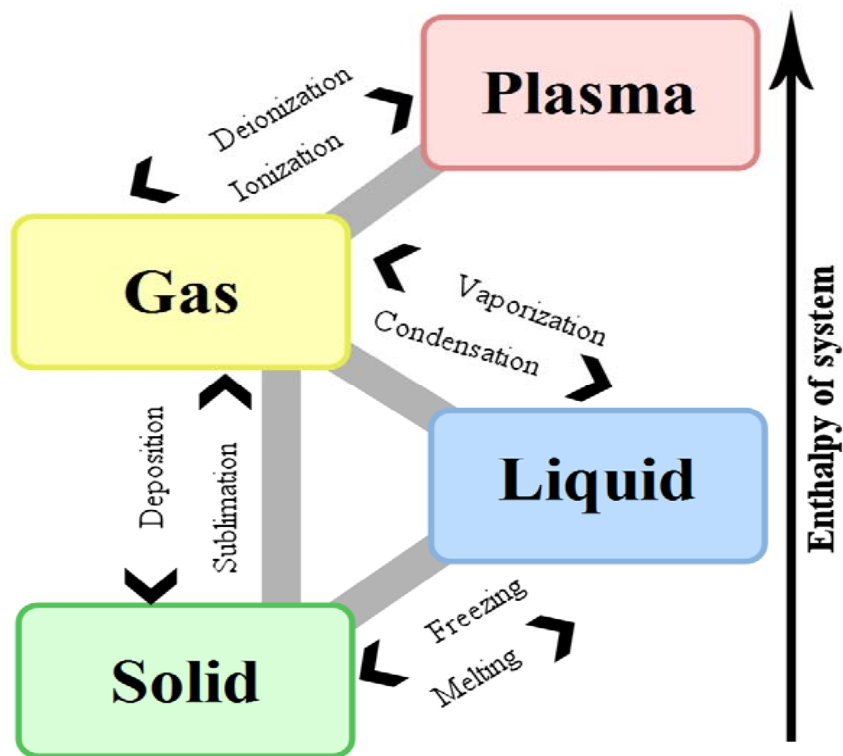


States of matter

1. States of matter
2. Gas state
3. Gas laws
4. Liquid state
5. Properties of liquids, surface forces
6. Solid state
7. Crystal lattices
8. Plasma state



States of matter



http://en.wikipedia.org/wiki/File:Phase_change_-_en.svg

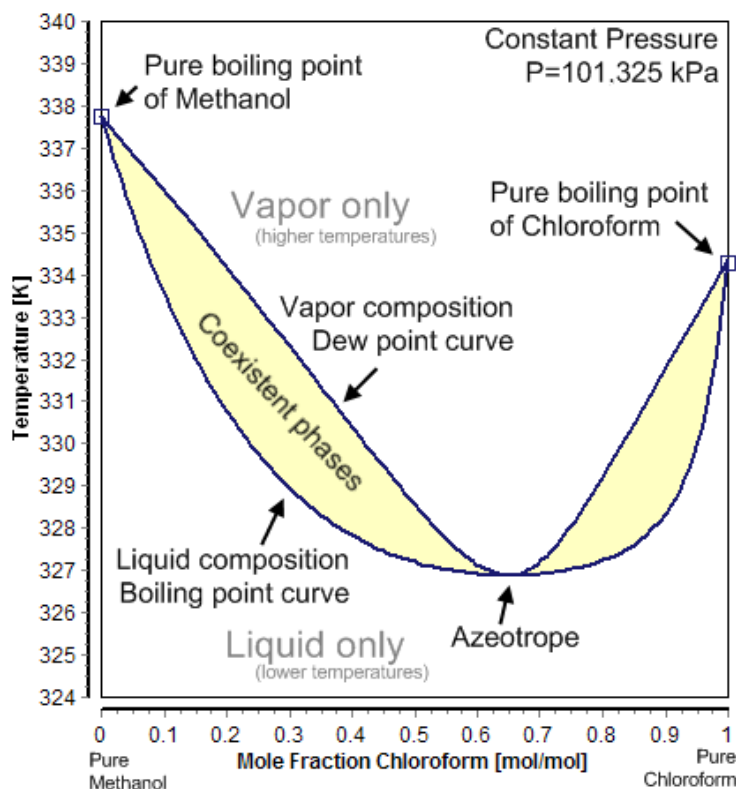


Solutions, mixtures

1. mixtures
2. miscibility
3. solubility
4. azeotropes, eutectic systems
5. colligative properties
 - lowering of vapor pressure
 - freezing point depression, boiling point elevation
 - osmosis pressure



Solutions, mixtures



T-x diagram of a minimum azeotrope chloroform and methanol

http://en.wikipedia.org/wiki/File:Positive_Azeotrope.png

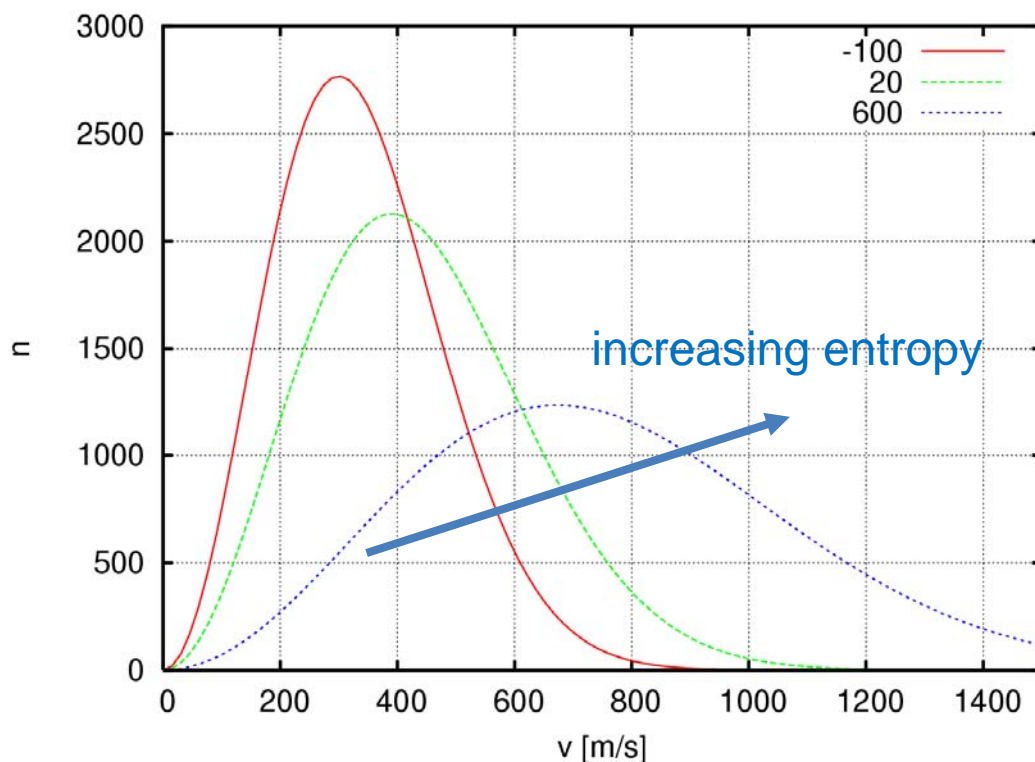


Thermodynamics

1. Laws of thermodynamics
2. Chemical thermodynamics
3. Extensive and intensive quantities
4. Heat
5. Entropy
6. Enthalpy
7. Gibbs free energy
8. Equilibrium



Thermodynamics



speed distribution of
of 1 million gas
molecules
at -100, 20 and
600 degrees °C

http://it.wikipedia.org/wiki/File:Maxwell-Boltzmann_distribution_1.png

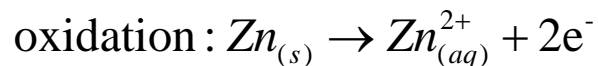
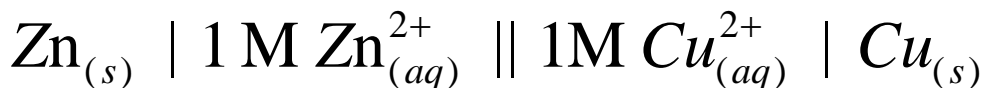




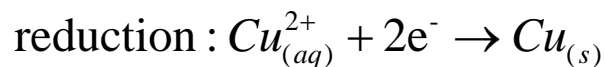
Electrochemistry

1. Electrolytes
2. Electrochemistry
3. Concentration cells
4. Galvanic cell
5. Electromotive force
6. Standard electrode potentials
7. Redox reactions
8. Electrolysis

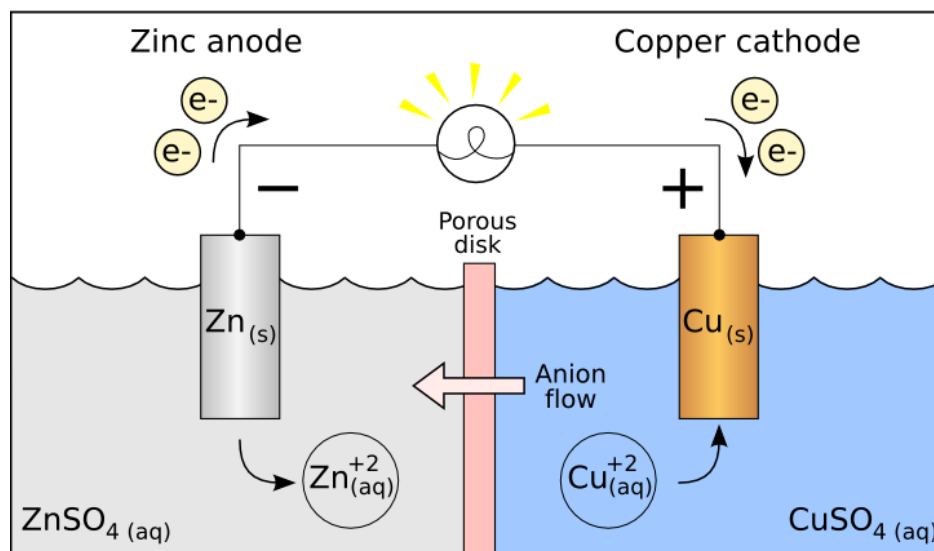
Electrochemistry



ANODE



CATHODE



http://en.wikipedia.org/wiki/File:Galvanic_cell_with_no_cation_flow.png